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Future Shapes of What's to Come

The Director's Corner

Steve Adamec
NAVO MSRC Director

The title for this issue of the *Navigator* says it all–"Future Shapes of What's to Come..." The NAVO MSRC is undergoing a carefully planned series of enhancements which, when completed in summer 2000, will provide one of the most capable, productive, and balanced high performance computing (HPC) environments in the world. These enhancements substantially boost the MSRC's computational capabilities across the primary HPC architectures we support—distributed-memory parallel, shared memory, and parallel vector. The enhancements also boost the mass storage and networking capabilities of the MSRC as well.

The most successful and requested HPC system within the NAVO MSRC, the Cray T3E, has been expanded by 33 percent to 1,088 processors and approximately 400 GB of aggregate memory. A new IBM RS/6000 SP system with 1,336 POWER3/375 processors and 1.3 TB of aggregate memory, one of the largest systems ever built by IBM, is being installed as this issue goes to press. Both the Cray T3E and the IBM SP are intended to provide the premiere, high-end computational environment for applications throughout Department of Defense (DoD) that simply cannot be run on lesser systems—applications that typically run as DoD challenge projects. To supplement this enormous distributed-memory parallel computational capability, we have installed a Sun HPC10000 computational server with 64 processors and 64 GB of shared memory—a unique resource which primarily supports interactive shared-memory HPC work and diagnosis/debugging work for large parallel applications. The SGI Origin 2000 systems (now known formally as the SGI 2800) have been merged and expanded to a single 256-processor system running a single IRIX image, greatly enhancing their capability to support shared-memory Challenge project work. The Cray T932 will be retired at year's end, with two additional Cray SV1 system nodes (for a total of four) being added to the existing Cray SV1 system. The upgraded SV1 will be configured with 4 gigawords (i.e., 32 GB) of shared memory—the largest memory ever offered on a parallel vector system at the NAVO MSRC. Finally, the internal mass storage and networking capabilities of the MSRC have been completely reengineered for performance and resiliency, providing a perfect fit with our new OC-12 wide-area Defense Research and Engineering Network (DREN) connectivity.

We invite you, the DoD user community, to let us assist you in utilizing this cutting-edge capability in support of your HPC needs.

About the Cover:
Future shapes of what's to come...The US Army's Theater High Altitude Area Defense Interceptor (THAAD) is a finless missile that utilizes ten liquid bi-propellant divert and attitude control jets for maneuvering during acquisition and homing of an incoming target. Through extensive use of Computational Fluid Dynamics (CFD), researchers have been able to generate engineering and aerodynamic data that would otherwise not have been available for the development and checkout of the THAAD missile (see story on page 12).

The Naval Oceanographic Office (NAVO) Major Shared Resource Center (MSRC): Delivering Science to the Warfighter

The NAVO MSRC provides Department of Defense (DoD) scientists and engineers with high performance computing (HPC) resources, including leading edge computational systems, large-scale data storage and archiving, scientific visualization resources and training, and expertise in specific computational technology areas (CTAs). These CTAs include Computational Fluid Dynamics (CFD), Climate/Weather/Ocean Modeling and Simulation (CWO), Environmental Quality Modeling and Simulation (EQM), Computational Electromagnetics and Acoustics (CEA), and Signal/Image Processing (SIP).

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Summary of Links Found Inside

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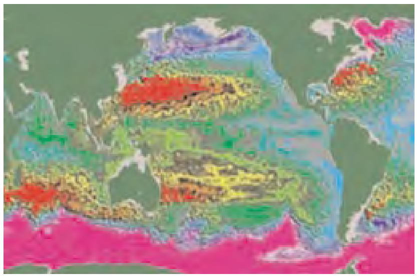
A Global Ocean Nowcast/Forecast System

Harley E. Hurlburt and Alan J. Wallcraft, Naval Research Laboratory (NRL)



Project:
Global and Basin-Scale Ocean Modeling and Prediction

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Assigned Site/System:
NAVO MSRC SGI/Cray T3E

CTA:
Climate/Weather/Ocean Modeling and Simulation

URL:
http://www7320.nrlssc.navy.mil/global_nlom/index.html

This project is aimed at developing an ocean prediction system that will revolutionize the ability to nowcast and forecast the global ocean circulation down to the scale of oceanic fronts and eddies. A real-time demonstration for the Pacific Ocean is currently running in real time at NAVO MSRC with 1/16° resolution, a demonstration that will be expanded to the global ocean in the near future. Department of Defense (DoD) High Performance Computing (HPC) resources and DoD HPC Challenge projects at NAVO MSRC and U.S. Army Engineer Research and Development Center (ERDC) MSRCs have been critical to this effort.

INTRODUCTION

DoD HPC and a DoD HPC Challenge grant on the NAVO MSRC SGI/Cray T3E are critical components of a coordinated 6.1-6.4 Naval Research Laboratory (NRL) effort on the "Grand Challenge" problem of eddy-resolving global ocean modeling and prediction. The goal is a fully eddy-resolving, data assimilative global ocean prediction system with at least 1/16° (~7.5 km) resolution in the near term, with an upgrade to 1/32° when the available computer power is sufficient. A 1/16° system is currently running in demonstration mode for the Pacific north of 20°S, and expansion to the global ocean is planned in the near future using DoD HPC Challenge resources at the NAVO MSRC and the NRL Layered Ocean Model (NLOM).

The 1/16° Pacific NLOM system already gives a real-time view of the ocean down to the 50-200 km scale of ocean eddies and the meandering of ocean currents and fronts, a view with unprecedented resolution and clarity. This can be seen at the URL. The system has demonstrated forecast skill for a month or more for many ocean features, including the fronts and eddies. The assimilation of satellite altimeter data into this system makes effective use of the near-real-time altimeter data from TOPEX/POSEIDON and ERS-2 that is available from Naval Oceanographic Office's (NAVOCEANO's) Altimetry Data Fusion Center (ADFC). The effectiveness of the model assimilation of altimeter data is greatly enhanced by the 1/16° resolution of the Pacific system, as demonstrated by comparison to corresponding results at coarser resolution. Other data, such as sea surface temperature and sparse vertical profiles of temperature and salinity, will be assimilated as well.

BACKGROUND

Ocean forecasting is in principle similar to atmospheric forecasting, but with two major complications: (a) ocean eddies, at about 100 km across, are typically 20 to 30 times smaller than comparable atmospheric highs and lows which means that roughly four orders of magnitude more computer time and three orders of magnitude more computer memory are required; and (b) there are relatively few observations below the ocean surface, so data assimilation is effectively confined to using satellite observations of the surface. The duration of forecast skill for the ocean is not restricted to the 10- to 14-day limit for atmospheric highs and lows. We have demonstrated at least 30-day predictive skill for ocean eddies and the meandering of ocean currents and fronts, given sufficient ocean model resolution and satellite altimeter data from TOPEX/POSEIDON and ERS-2.

A major component of NRL's ocean modeling program has been a detailed study of the resolution required for ocean prediction. We have strong evidence that NLOM and other ocean models (including all the popular global and basin-scale ocean models) need to use grid cells for each prognostic variable that are at most about 8 km across at mid-latitudes. Our research has shown that doubling the resolution to 4 km per cell gives substantial improvement but doubling again to 2 km gives only modest additional improvement. Due to ocean modeler preference and choice of finite difference grid design, there is significant variation in how such resolution is expressed in degrees, the most common way to describe ocean model resolution. For the NLOM grid it translates to 1/16°, 1/32°, and 1/64° resolution, respectively. This is for the global and basin-scale. Coastal models would use the global forecast

for boundary conditions and would require much smaller cells, but would cover only a limited region.

At 4 km, the optimal resolution is finer than might be expected based on the size of eddies. In relation to ocean eddy size, it is similar to the resolution currently used by the leading weather forecasting models in relation to the size of atmospheric highs and lows. More specifically, our research has shown that fine resolution of the ocean eddy scale is required to obtain coupling between upper ocean currents and seafloor topography via turbulent flow instabilities. This coupling can strongly affect the pathways of upper ocean currents and fronts, including the Gulf Stream in the Atlantic and the Kuroshio in the Pacific. The high resolution is also required to obtain sharp fronts that span major ocean basins and a nonlinear effect on the large scale C-shape of ocean gyres, such as the Sargasso Sea in the Atlantic.

TECHNICAL APPROACH

As far back as 1989, the President's Office of Science and Technology recognized global ocean modeling and prediction as a "Grand Challenge" problem, defined as requiring a computer system capable of sustaining at least one trillion floating point adds or multiplies per second. By taking a multi-faceted approach to cost minimization, we are solving the problem on systems capable of only a small percent of this performance. One facet is experiment sequences that use the largest cell size possible and an ocean basin rather than the entire globe whenever possible. This only gets us so far, since in the end there is no substitute for small cells and a global domain.

Another facet is the use of the NLOM which has been specifically designed for eddy-resolving global ocean prediction. It is tens of times faster than other ocean models in computer time per model year for a given horizontal resolution and model domain. NLOM's performance is in turn due to a range of design decisions, the most important of which is the use of isopycnal (density tracking) layers in the vertical rather than the more usual fixed depth cells. Density is the natural vertical coordinate system for the stratified ocean, and it allows seven NLOM layers to replace the 100 or more fixed levels that would be needed at 1/16° resolution. Another important advantage of this approach is that there is less need to increase the number of density tracking layers as the horizontal cell size is reduced. With NLOM, halving the cell size requires about 8 times as much computer power (4 times from the number of cells plus 2 times from the required smaller time step), but with fixed-level ocean models, the number of cells in the vertical should also be doubled, requiring about 16 times as much computer power.

A third facet is a widely portable NLOM computer code, developed under the Common High Performance Computing Software Support Initiative (CHSSI) program, that targets large scalable computers with high-speed network connections. NLOM exhibits very good scalability (wall time speedup as more processors are used) on such systems. For example, we have routinely run NLOM on up to 1,152 Cray T3E processors at up to a sustained speed of about 100 billion useful floating-point operations per second.

A final facet of our efficiency drive is the use of an inexpensive data assimilation scheme backed by a statistical technique for relating surface data to subsurface fields. The statistics are from an atmospherically forced 20-year inter-annual simulation of the same ocean model, an application that requires a model with high simulation skill.

So far it has been possible to run NLOM in demonstration mode with 1/32° resolution globally (72°S-65°N) and 1/64° resolution over the basin-scale subtropical Atlantic (9°N-51°N), including the Caribbean and Gulf of Mexico. While, at present, these require greater computer resources than practical for an operational product, they do give information on the value added of increasing resolution and insight into model performance at 1/16° resolution.

RESULTS

In August 1999, we started running 1/16° Pacific NLOM in near-real time (i.e., updated every few days). In hindcast studies that followed standard nowcast and forecast procedures, but used data from a previous time period, we compared 1/16° Pacific NLOM with 1/4° global NLOM. Both studies assimilated satellite altimeter data from TOPEX/POSEIDON and ERS-2, and then

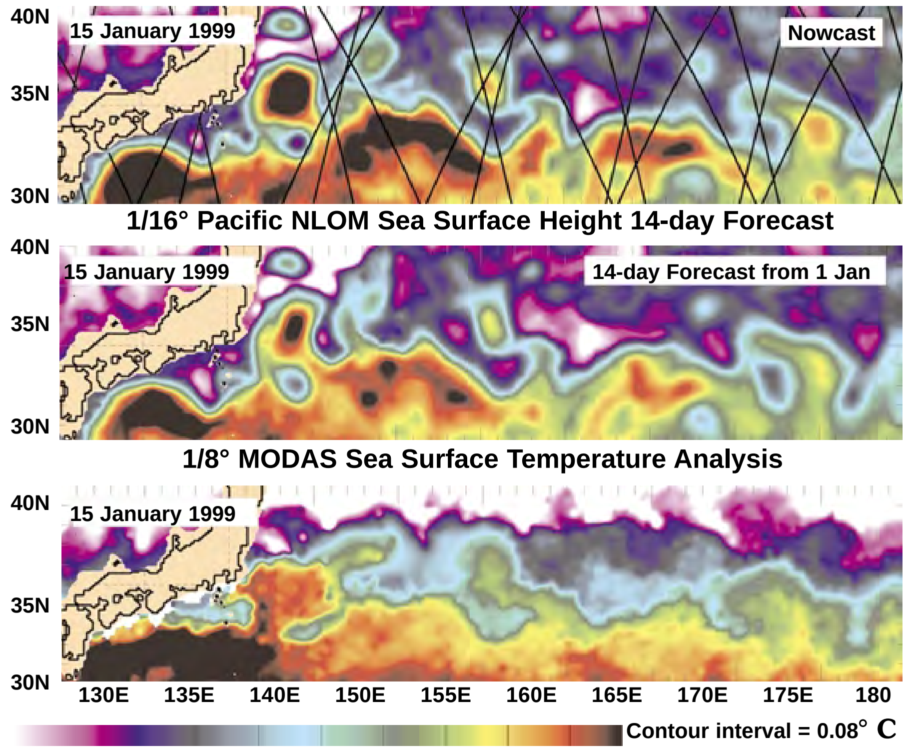


Figure 1. Zoom on the Kuroshio current region south and east of Japan. (Top) Sea surface height (SSH) for 15 January 1999, from the NRL 1/16° Pacific model with assimilation of satellite altimeter data from TOPEX/POSEIDON and ERS-2. The altimeter tracks with data available for this update cycle are overlain. (Middle) Corresponding SSH snapshot from a 14-day forecast initialized from 1 January 1999. (Bottom) MODAS 1/8° SST analysis from satellite IR imagery. The SST color bar is designed to highlight the Kuroshio pathway.

month-long forecasts started from the data assimilative nowcast states were performed. An example is shown in Figure 1 with comparison to an independent 1/8° SST analysis from the Modular Ocean Data Assimiltion System (MODAS) that is operational at NAVOCEANO. The SST analysis shows the correspondence between the Kuroshio pathway and some of the eddies seen in the sea surface height field from the Pacific Ocean model, a field observed by satellite altimetry as shown by overlain ground tracks in Figure 1 (top panel).

The 1/16° Pacific model has given the very first basin-wide skillful forecast demonstration of oceanic fronts and eddies for any ocean basin. The Pacific results also demonstrate that altimeter data alone are sufficient to produce an accurate nowcast when a high resolution ocean model is in the loop to fill in the space-time gaps in the altimeter data. The 1/4° global model was much less successful in this feasibility demonstration, as was expected from the earlier discussion of resolution requirements. In addition, the nowcast/forecast results at 1/16° resolution were substantially better than expected for a system that uses satellite altimeter data as the only observing system, due mainly to doubts about the space-time resolution adequacy of the altimeter data. SST assimilation will be added in the near future.

The global results for SST have also exceeded expectations, particularly for a model with only seven layers in the vertical. The embedded mixed layer in NLOM gives accurate SST based on accurate atmospheric forcing even with no assimilation of SST data (or altimeter data). With climatological atmospheric forcing, global NLOM gives SSTs accurate to within .5°C for the annual mean and .7°C for the seasonal cycle. Global NLOM at 1/2° and 1/8° resolution was run 1979-98 with 6-12 hourly atmospheric forcing from ECMWF and no assimilation of SST data, and then compared to 337 year-long daily time series of observed SST around the world over the 1980-98 time frame. The median rms error was .8 to .9°C and the median correlation coefficient was about .9, again with no assimilation of SST data. The modal bin for rms error was .6 to .8°C, and the modal bin for correlation was .95 to 1.0.

Figure 2 shows similar results from 1/16° Pacific NLOM, but with a comparison between results using Fleet Numerical Meteorology and Oceanography Center (FNMOC) Navy Operational Global Atmospheric Prediction System (NOGAPS) and European Centre for Medium-Range Weather Forecast (ECMWF) winds over the time frame 1990-1998. In both cases ECMWF thermal fields were used because such fields are not available from FNMOC prior to late 1997. However, the winds play a significant role in thermal forcing, and the FNMOC winds were used for that purpose in the FNMOC forced run. As before, there was no assimilation of SST data. In both cases the median rms SST error was .84°C, but outside the equatorial region the SST results using FNMOC were noticeably better, .76°C vs. .84°C, using ECMWF, with median correlation of .96 and .95, respectively. Note the three years of daily SST in Figure 2 show substantial differences in the shape of the annual cycle as well as shorter time-scale variability that is captured by the NLOM SSTs, an indication of skill for both the ocean model and the atmospheric forcing.

These results indicate that NLOM SST is sufficiently accurate to be used as a platform for assimilation of SST data (which has gaps due to cloudiness) and for SST forecasting.

Acknowledgments

This work is a contribution to the 6.2 Basin-scale Ocean Prediction System project funded by the Office of Naval Research under program element 62435N and to the 6.4 projects Large Scale Ocean Modeling and Ocean Data Assimilation funded by the Space and Naval Warfare Systems Command under program element 63207N. The numerical model was run on SGI/Cray T3Es at the Naval Oceanographic Office, Stennis Space Center, Mississippi and at the U.S. Army Engineer Research and Development Center, Vicksburg, Mississippi. Both are part of the Defense Department's High Performance Computing Initiative.

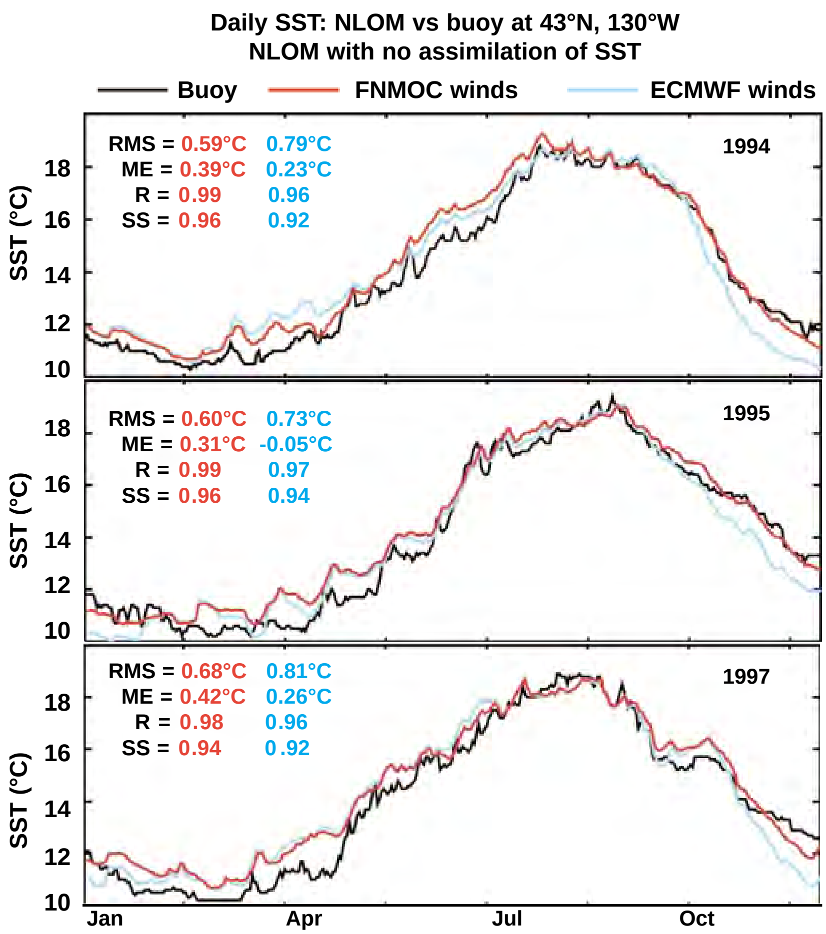


Figure 2. Daily observed SST from a NOAA buoy at 43°N, 130°W (black) and modeled SST from 1/16° Pacific NLOM forced with 6-12 hourly winds from FNMOC NOGAPS (red) and the ECWMF (blue) for 1994 (top), 1995 (middle), and 1997 (bottom). Thermal forcing (except the wind component) is from ECMWF in both cases. NLOM included no assimilation of SST data. Statistics include root mean square error (RMS), mean error (ME), correlation (R), and skill score (SS).

Large-Scale Atom Simulation

Dr. Rajiv K. Kalia, Louisiana State University

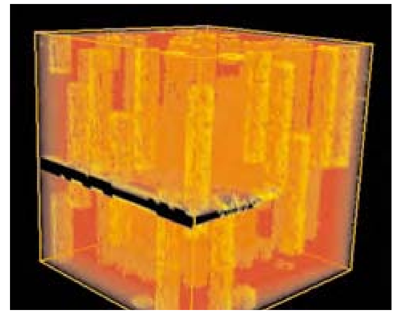
Novel materials that can withstand high temperatures and extreme environments are generating considerable worldwide attention. Such materials are tremendously important for defense technologies. The basic requirements for designing materials that have low densities, elevated melting temperatures, high oxidation and corrosion resistance, the ability to resist creep, and high toughness encompass some of the most challenging problems in materials science.

With this DoD Challenge grant, we have performed large-scale (106-108 atoms) molecular dynamics (MD) simulations to investigate dynamic fracture in ceramics and nanocomposites and dynamics of oxidation of metallic nanoparticles. These simulations have been executed with highly efficient, portable and scalable, multiresolution algorithms including the fast multipole method for the long-range Coulomb interaction, a dynamic load-balancing scheme for mapping irregular applications on parallel machines, and a fractal-based compression scheme for scalable I/O and data communication.

DYNAMIC FRACTURE IN CERAMICS AND NANOCOMPOSITES

Molecular dynamics simulations were performed to investigate dynamic fracture in crystalline SiC and GaAs at various temperatures using 256 nodes of Cray T3E at the NAVO MSRC. The simulations were carried out on a thin-strip sample for which the mechanical energy release rate, G, can be calculated from the knowledge of the applied strain, e, and the value of the stress, s, far ahead of the crack tip: G = Wse/2. In addition to the mechanical energy release rate, the crack-tip velocity and local stress distribution at various temperatures were monitored. Figure 1 shows the results of 30-million-atom MD simulations of SiC at room temperature and 1,500K. We find that large shear stresses close to the crack tip cause cleavage fracture at room temperature. At elevated temperatures, dissipative effects due to dislocations, micropore formation and coalescence, and crack deflection cause stresses to spread out all over the system, thereby increasing the value of G.

Similar effects are observed in our 100-million atom fracture simulations



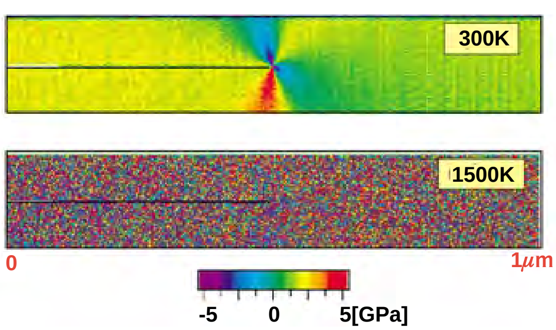


Figure 1. Shear stress distributions in 30 million atom MD simulations of SiC at 300K and 1500K.

Project:

Computational Assisted Development of High Temperature Structural Materials

Principal Investigators:

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Assigned Site/System:

NAVO MSRC SGI Origin

CTA:

Computational Chemistry and Materials Science

URL:

http://www.cclms.lsu.edu/cclms/research/research-nanophase.html

of GaAs. The MD results also indicate that the brittle-to-ductile transition temperature in GaAs (~ 600K) is close to the experimental value (630-660K). Figure 2 shows snapshots of three different crack fronts in MD simulations of GaAs at room temperature.

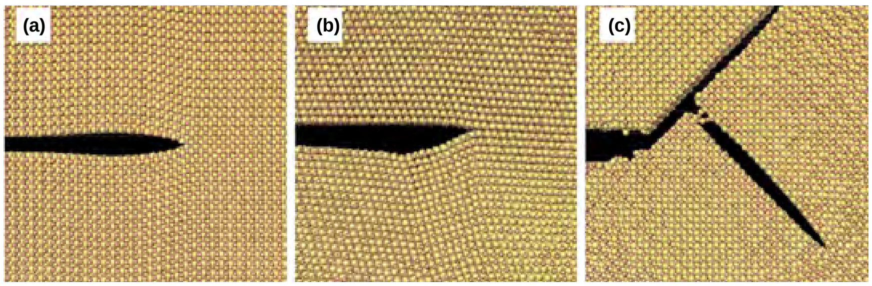

Figure 2. Snapshots of cracks in MD simulations of GaAs. Crack surfaces are (a) (110), (b) (111), and (c) (001).

One of the most promising materials for high-temperature structural applications is a fiber-reinforced ceramic composite of silicon nitride host embedded with fibers of silicon carbide. The fibers are coated with materials that form weak interfaces between fibers and the matrix. We have performed 10 million atom MD simulations to investigate the effect of interphase structure and residual stresses on fracture toughness in a silicon nitride matrix reinforced by silicon carbide fibers coated with amorphous silica layers (see Figure 3). Immersive visualization of these simulations reveals a rich diversity of atomistic processes including fiber rupture, frictional pullout, and emission of molecular fragments, which must all be taken into account in the design of tough ceramic composites.

DYNAMICS OF OXIDATION OF ALUMINUM NANOCLUSTERS

Dynamical oxidation simulations were motivated by experiments that reveal unique electrical, optical, and mechanical properties of nanocomposites consisting of passivated Al nanoparticles. This led us to perform the first successful MD simulation of oxidation of an Al nanocluster using MD simulations based on a highly reliable interaction scheme that can successfully describe a wide range of physical properties of both metallic and ceramic systems. This scheme includes changes in charge transfer as the atoms move and is thus capable of treating bond formation and bond breakage. Dynamic charge transfer gives rise to computationally intensive Coulomb interaction which, for the number of atoms necessary in a realistic simulation, requires highly efficient algorithms that map well onto parallel architectures. The fast multipole method (FMM) of Greengard and Rokhlin was used to reduce the computational complexity from O(N2) to O(N) for the long-range Coulomb interaction with extensions for stress calculations. A multiple time-step algorithm further reduced the execution time by an order of magnitude. Both algorithms map very well onto parallel architectures.

Dynamic oxidation simulations reveal a rapid three-step oxidation process culminating in a stable oxide scale in 50 ps. In the first 5 ps, oxygen molecules dissociate, and the oxygen atoms first diffuse into octahedral and subsequently into tetrahedral sites in the nanoparticle. In the next 20 ps, as the oxygen atoms diffuse radially into and the Al atoms diffuse radially out of the nanoparticle, the fraction of six-fold coordinat-

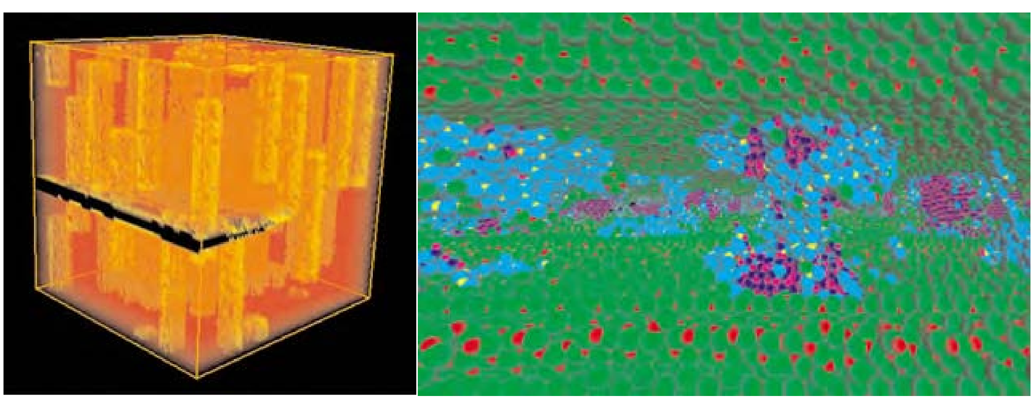

Figure 3. (Left panel) Fractured silicon nitride (red) ceramic reinforced with silica-coated carbide fibers (yellow). (Right panel) Close-up of the fractured composite system. Small spheres represent silicon atoms, and large spheres represent nitrogen (green), carbon (magenta), and oxygen (cyan) atoms.

ed oxygen atoms drops dramatically. Concurrently, there is a significant increase in the number of O atoms that form isolated clusters of corner-sharing and edge-sharing OAl4 tetrahedra. Between 30 and 35 ps, clusters of OAl4 coalesce to form a neutral, percolating tetrahedral network that impedes further intrusion of oxygen atoms into and of Al atoms out of the nanoparticle (see Figure 4). As a result, a stable oxide scale is formed. Structural analysis reveals a 40 Å thick amorphous oxide scale on the Al nanoparticle. The thickness and structure of the oxide scale are in accordance with experimental results.

Currently we are planning multiscale simulations to determine residual stresses, fracture toughness and hardness, friction and adhesion, and material degradation due to oxidation in: (1) polydimethylsiloxane (PDMS) on alumina and silica surfaces; (2) nanostructured composites consisting of aluminum nanoparticles passivated with oxygen; (3) Al/Al2O3, Al/SiC, and Ti/TiO2 metal/ceramic interfaces; and (4) functionalized atomic-force microscope (AFM) tips of silicon nitride and carbon nanotubes.

These Challenge applications require a methodology that can describe physical and chemical processes over several decades of length scales. Quantum mechanical (QM) simulations based on the density function theory (DFT) are performed in regions where atomic bonds are formed or broken; molecular dynamics (MD) simulations are carried out in non-linear regions surrounding the QM region; and the finite-element (FE) approach with constitutive input from QM or MD calculations is used in regions far away from the process zones. The QM, MD, and FE schemes are integrated with an approach based on control theory. Algorithms will be designed to carry out these hybrid QM/MD/FE simulations in DoD's metacomputing environment with multiple parallel machines, mass storage devices, and immersive and interactive virtual environments on a grid with high-speed networks.

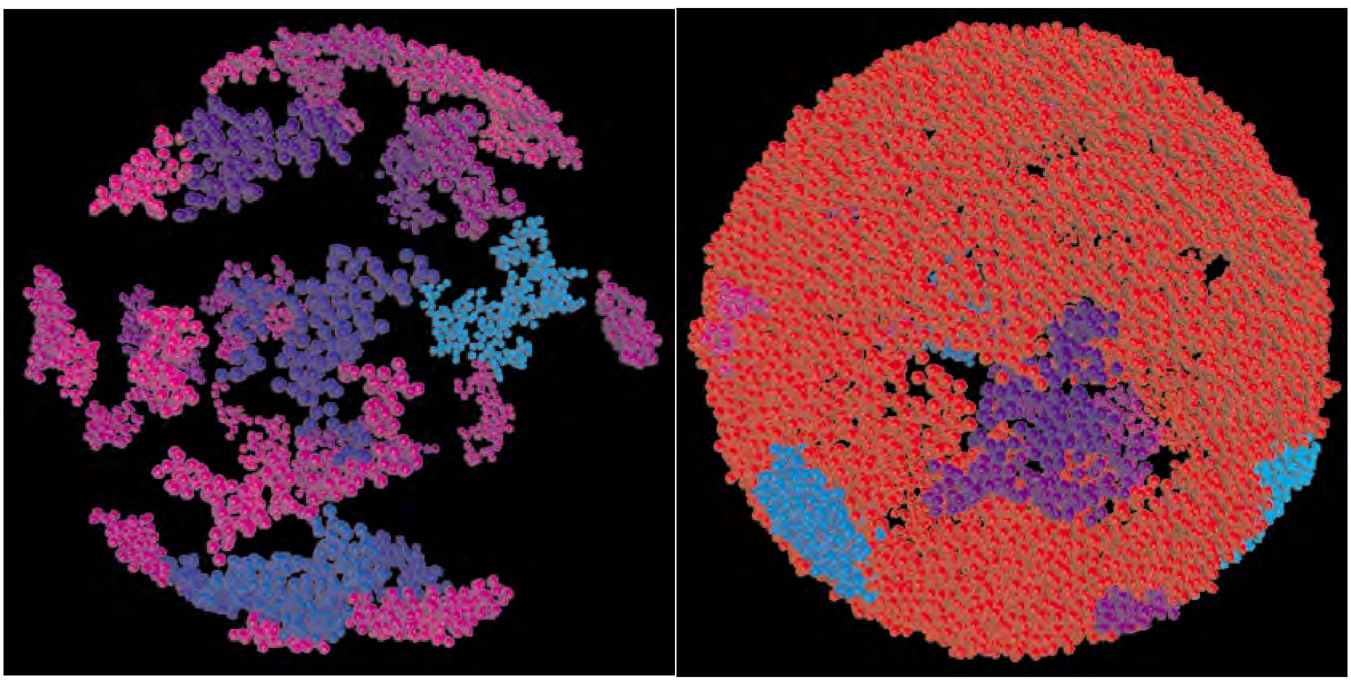

Figure 4. Initial stage of oxidation of an A1 nanoparticle. Size distributions of $OA1_4$ clusters at 20 ps (left) and 31 ps (right) are shown. Clearly, the clusters coalesce and percolate rapidly.

Dynamic Visualizations

Dr. Robert Moorhead, Director VAIL, Mississippi State University

The scientific visualization group at Mississippi State University's National Science Foundation (NSF) Engineering Research Center (ERC) for Computational Field Simulation has long been associated with NAVO MSRC. Dr. Robert J. Moorhead II, Director of ERC's Visualization, Analysis, and Imaging Laboratory (VAIL)(http://www.erc.msstate.edu/labs/vail/) and his group have worked with NAVO MSRC since 1991. Highlights of VAIL's visualization work targeted at the METOC community include three packages: Interactive Structured Time-varying Visualizer (ISTV) (http://www.erc.msstate.edu/research/thrusts/scivi/html/ISTV), the EnVis toolkit, and the CTHRU virtual environment.

STV

ISTV is an X/Motif application (see figure 1) using OpenGL graphics to support interactive visualization of a wide variety of model data on desktop workstations and larger machines. Although primarily targeted at geospatial datasets, it can be used with any 3D (static or time-varying) structured data. ISTV's use of logical grid files (LGFs) for data description and organization allows users to specify computational grid parameters implicitly (in the case of regular latitude/longitude grids commonly employed in METOC simulations) without the need to create large grid files to complement the simulation solutions.

ISTV supports the simultaneous visualization of model output from several independent sources, without regard to differences in the sampling frequencies of the various grids (see figure 2). This capability allows users to examine relationships between forcing fields (e.g., wind data) and the output of ocean circulation models.

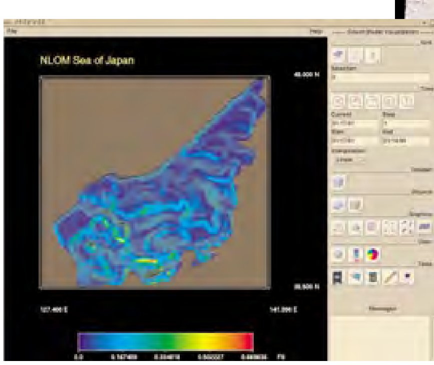

Figure 1

The inherent size of basin-scale ocean models makes intelligent data handling a crucial part of the system. In many cases, we cannot expect to read the entire grid or solution set into main memory. Instead, ISTV allows the user to subsample large datasets before reading; the user can also combine this with reading only a selected region of interest to further limit the memory requirements of the visualization. A fixed amount of memory is used as a local buffer to enhance the interactive speed of the system.

A calculator module is available to compute derived values, as they are needed. Many simple operations already exist in the calculator, and more complex or domain-specific computations can be added to the code. When animating, data are linearly interpolated along the time axis from the two adjacent time steps. All data derivation and interpolation operations handle invalid values like "land masks" found in many ocean model data sets.

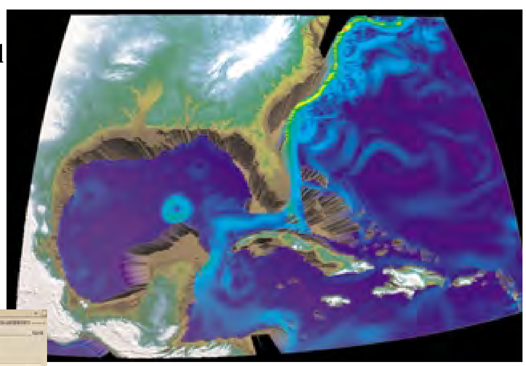

Figure 2

An important design consideration in ISTV is the ability to work with data in its native file format. Converting to a new format is costly and problematic, so ISTV does not require this. The code was designed so that a reader for a new file format could be integrated with a minimal amount of effort.

Normally ISTV runs as a single job on a single computer. Quite often, however, the data files reside on a central file server rather than on the visualization machine. In this case, ISTV has a data server/visualization client option in which each task executes on the appropriate machine; network communication between the data server and front-end visualization client is managed by message passing interface (MPI).

ENVIS TOOLKIT

The EnVis toolkit is built upon the COST (Common Object Software Toolkit) framework developed at the ERC to provide a common code base for the development of scientific visualization tools. Initial development focused on providing interactive visualization tools, but with the rapid increase in model resolutions, we also added batch-mode visualization capabilities.

Since the machines serving datasets often contain no host-based graphics subsystems, we have moved from using OpenGL-based rendering to either using offscreen-rendering capabilities provided by the Mesa graphics library http://mesa3d.sourceforge.net or other software-only rendering techniques. We

have used our Mesa-enabled offscreen renderer on the NAVO MSRC Origin 2000 machines and are now engaged in porting the toolkit to Solaris for use on both multiprocessor Sun machines as well as networks of Sun workstations (see Figure 3).

CTHRU

CTHRU, a virtual environment first developed at the ERC for the Supercomputing 1995 conference, has been enhanced with new features in the past year. Originally designed to demonstrate the computational steering of a running NLOM ocean model from a visualization front-end using a CAVE, more recent uses of the system have focused on support for other models (e.g., NCOM Chesapeake Bay circulation model).

New features include a vertical cutting plane, which the user can interactively place, and menu items for changing level-of-detail subsampling rate, isosurface threshold, and layer selection (see Figures 4-6). Since current applications use host-based datasets, CTHRU's performance has also been improved for running on a single machine by using the native SGI MPI libraries which use shared memory as opposed to sockets for data communication.

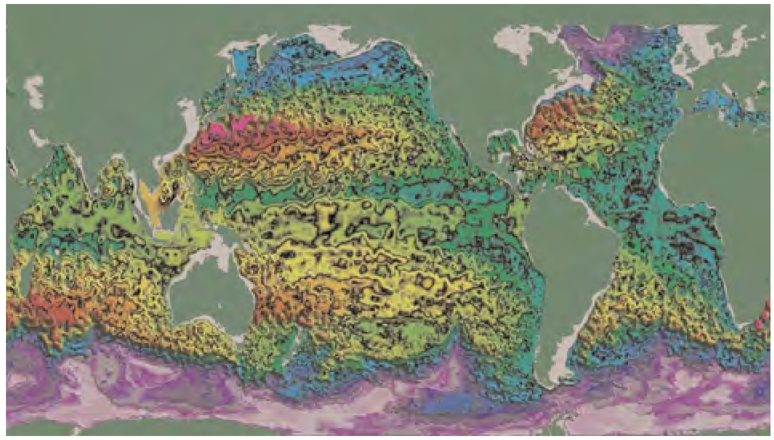

Figure 3

In addition to development of tools, VAIL tries to help the NAVO MSRC Visualization Lab by evaluating visualization toolkits developed elsewhere. Recently students, some of whom work in the NAVO MSRC Visualization Lab when they are not in school, have been evaluating the visualization of METOC data with the new open-source release of Data Explorer http://www.opendx.org/ and VisAD http://www.ssec.wisc.edu/~billh/visad.html, a Java-based visualization class library.

NOTE: Data are courtesy of the Naval Research Laboratory, and the use thereof does not constitute an endorsement.

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[2] C.W. Everitt, J. van der Zwaag, and R.J. Moorhead, "COST: Common Object Support Toolkit," C++ Toolbox, ACM SIGPLAN Notes, February 1998.

[3] K. Gaither, R. Moorhead, S. Nations, and D. Fox, "Visualizing Ocean Circulation Models Through Virtual Environments," IEEE Computer Graphics and Applications, Vol. 17, No. 1, January/February 1997, 16-19.

Figure 4

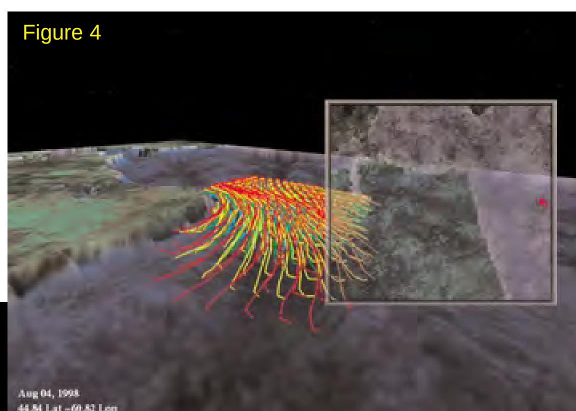


Figure 5

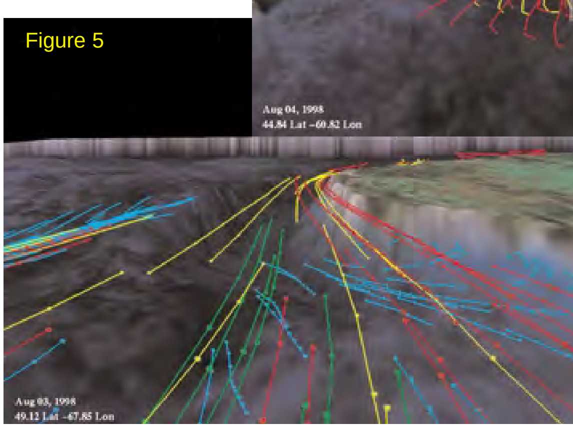
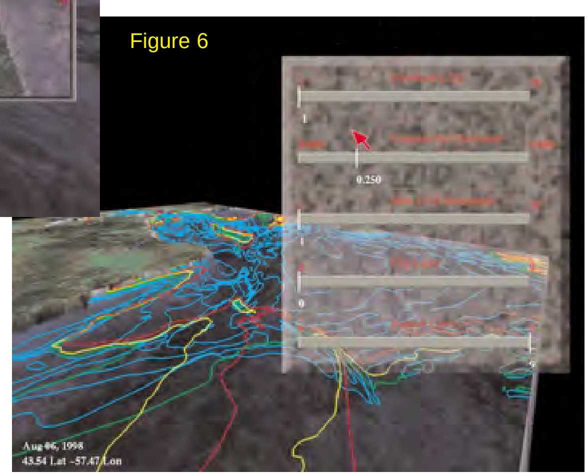


Figure 6



THAAD
Theater High Altitu

The U.S. Army's Theater High Altitude Area Defense Interceptor (THAAD) is a finless missile that utilizes ten liquid bi-propellant divert and attitude control jets for maneuvering during acquisition and homing of an incoming target. This type of control system generates aerodynamic interactions between the control jet exhaust and the oncoming flow that must be included in the autopilot design to achieve robust and reliable flight performance.

While extensive wind tunnel data have been collected from four tunnel entries for the development of appropriate guidance algorithms, these cold exhaust, subscale jet interaction (JI) data do not always simulate the true aerodynamics of an actual burning thruster at all altitudes.

Through extensive use of computational fluid dynamics (CFD), however, researchers have been able to generate engineering and aerodynamic data that would otherwise not have been available for the development and checkout of the THAAD missile. The data have been successfully utilized for improved design understanding, autopilot tuning and sensitivity studies, ground and flight test data analysis, and improved flight simulations. Each of the analyzed aspects of reaction jet control has contributed to an improved understanding of the missile aerodynamics and performance objectives, and greater confidence in the present design and future requirements has been achieved.

Encouraged by this success, THAAD is continuing to utilize HPC resources to examine additional aspects of JI phenomena before going to the next round of flight tests.

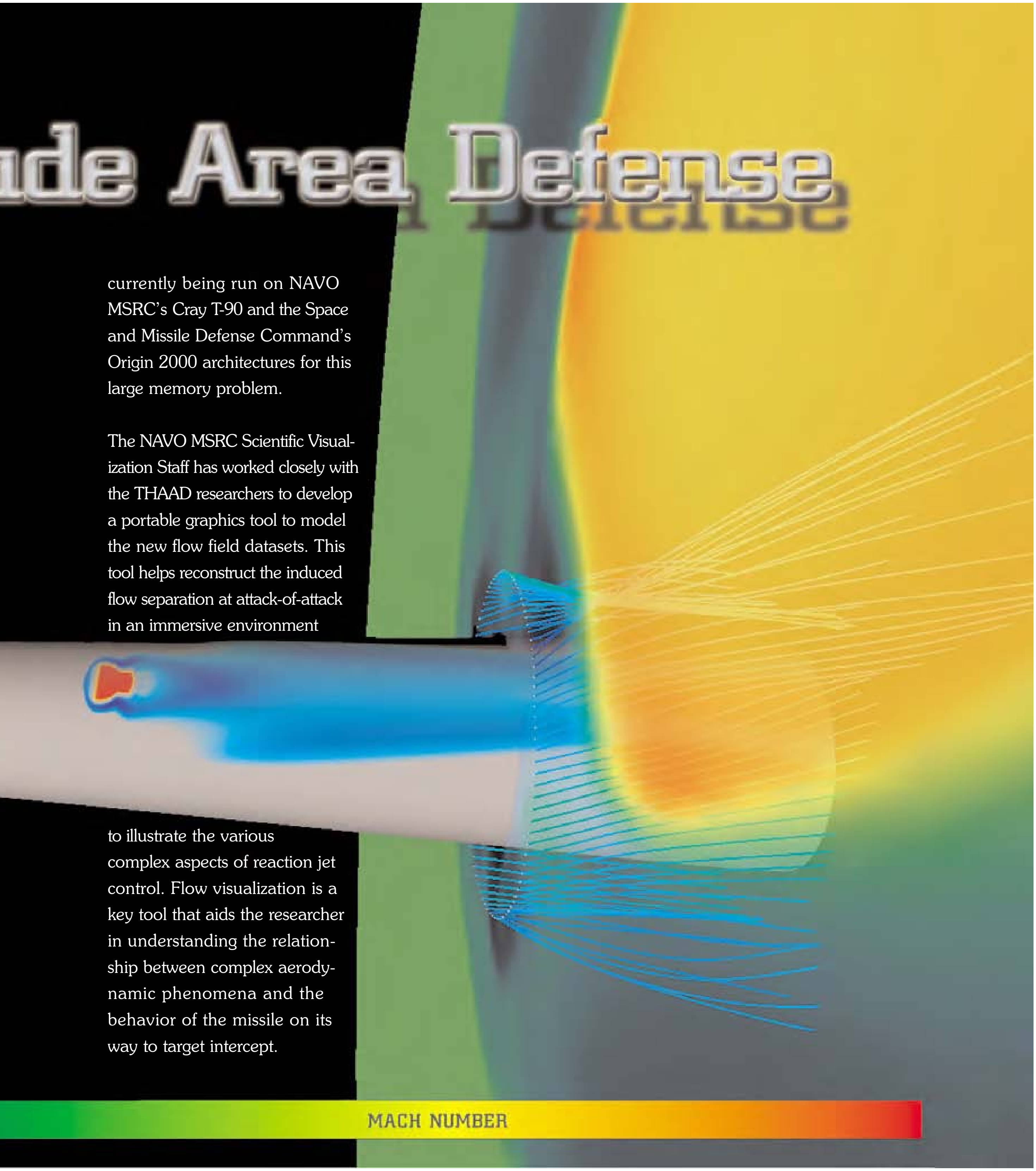
Current research is focused on the possible effects of hot jet exhaust flow over the infrared (IR) seeker window under certain flight conditions. A complete engineering design requires anticipation of software algorithms that may be necessary to acquire and

track dim targets, and it is wise to include any effects, no matter how slight, that may affect seeker performance. This aspect of the JI analysis is made more difficult by the high degree of computational grid resolution needed over a very large spatial domain for accurate simulation of the expanding jet flow. Computational simulations are

de Area Defense

currently being run on NAVO MSRC's Cray T-90 and the Space and Missile Defense Command's Origin 2000 architectures for this large memory problem.

The NAVO MSRC Scientific Visualization Staff has worked closely with the THAAD researchers to develop a portable graphics tool to model the new flow field datasets. This tool helps reconstruct the induced flow separation at attack-of-attack in an immersive environment to illustrate the various complex aspects of reaction jet control. Flow visualization is a key tool that aids the researcher in understanding the relationship between complex aerodynamic phenomena and the behavior of the missile on its way to target intercept.



FY 2000 PET Highlights

Eleanor Schroeder, NAVO MSRC Program Environment and Training Program (PET) Government Lead

The Annual PET Review was held the week of April 10th. As in previous reviews, there was a panel of external reviewers, consisting of people who have a broad background in high performance computing. Past reviewers have included Kay Howell (National Coordinating Office), Ann Hayes (Los Alamos National Laboratory), Bob Borchers (National Science Foundation), Valerie Taylor (Northwestern University), Charles Bender (Ohio Supercomputing Center), and Joan Novak (Environmental Protection Agency). Input from our external reviewers is invaluable to our programmatic and strategic planning efforts.

Our University of Virginia metacomputing project, Legion, is progressing well. We have been successfully interfacing with the Army Research Laboratory (ARL) folks and have set up and run a variety of tests. The "Legionization" of COAMPS is underway and on track. Oregon State is progressing on its Resource Allocation Tool. We are working through some security issues right now but hope to have everything resolved soon. San Diego Supercomputing Center is active on four tiger team projects. For more information about these and any of our projects, visit our web site: http://www.navo.hpc.mil/pet

We hosted several workshops in the first half of this year. A very successful Visualization Workshop was held in January that included participation from all four MSRCs. We held a well-attended seminar the day after the workshop on TeraMTA. We hosted the third annual Signal Image Processing Workshop, Unstructured Grids, and a Legion workshop. More information on these workshops can be found on our web site or by contacting Bob Melnik melnik@navo.hpc.mil .

We are currently soliciting proposals for our year 5 efforts. Please contact Walter Shackelford wshackel@navo.hpc.mil for more information. We plan to involve our Computational Technology Area leads in the review of our proposals again this year.

Scientific Visualization Workshop

Dr. Bob Melnik, CTA Coordinator

NAVO MSRC PET held its first Engineering and Scientific Data Visualization Workshop in January. Conducted in the NAVO MSRC PET classroom facilities, the workshop was attended by 26 participants, whose enthusiasm kept them working well into the evening on their lab exercises!

The purpose of the three-day workshop was to provide NAVO MSRC users with the information and skills needed to employ state-of-the-art visualization technology. Students were invited to "bring your data" to the workshop, which consisted of a mix of classroom lectures and hands-on laboratory exercises. The Army Research Laboratory (ARL), U.S. Army Engineer Researh and Development Center (ERDC), and NAVO MSRCs presented the activities of their respective visualization laboratories and participated in seminars on the state-of-the-art in scientific and engineering data visualization technology. The workshop concluded with a panel discussion of emerging developments in visualization technology.

For those who could not be present, workshop materials can be found at the NAVO MSRC web site: http://www.navo.hpc.mil/pet/viz2000

Two visualization packages, AVS 5 and Data Explorer, were presented in tutorials. Both are full-featured, state-of-the-art software systems that can produce professional quality visualizations of engineering and scientific data. The tutorials were given at an introductory level and were directed toward users with little experience in advanced visualization software packages.

AVS 5 is a fully supported commercial application for data visualization from Advanced Visual Systems of Waltham, MA. It is available for both Unix and Linux operating platforms. Data Explorer is a new open-source application that is evolving from an earlier commercial application known as "IBM Visualization Data Explorer." An organization known as OpenDX has been formed in cooperation with IBM to coordinate the development of an Open Source version of Data Explorer. Binary versions of Data Explorer for Windows, Unix, and Linux platforms are available for download, at no charge, from the OpenDX organization web site.

Additional information on AVS 5 and Data Explorer can be found at their organization's web sites:

AVS 5: http://www.avs.com/products/AVS5/avs5.htm

OpenDX: http://www.opendx.org

NAVO MSRC would be pleased to repeat the workshop in the future. If you desire to attend a visualization workshop in the future, please contact the NAVO MSRC PET Training Coordinator, Brian Tabor, at taborb@navo.hpc.mil .

PET Workshops

2000 Winter Legion Workshop

The joint Legion Group/Applied Metacomputing Winter 2000 Workshop was held in January at the University of Virginia. Participants received introductory information, started a system, ran applications, and learned advanced system administrative tasks in hands-on sessions. A second workshop was held in May. Both workshops were well attended by academic, government, and corporate participants and included information on customizing and troubleshooting systems. For more information on these workshops, visit

http://www.legion.virginia.edu/workshops.html

Dual-Level Parallelism and Multi-Block Grids and Coastal Ocean Circulation Modeling

This one hour workshop held in March introduced a multi-block grid generation technique and a dual-level parallel implementation into the Princeton Ocean Model (POM). MPI was used to parallelize the POM, assigning each grid block a unique processor. OpenMP dynamic threading was used to alleviate workload variations between MPI processes. Dr. Phu Luong, ERDC Environmental Quality Modeling and Simulation (EQM) On-site Lead, demonstrated the efficacy of the MPI-only and MPI/OpenMP code versions of the POM model on both a one-block and twenty-block grids. For more information, visit

http://www.navo.hpc.mil/cgi-bin/pet/Training/training.cgi/

Distributed Computing and Environmental Modeling Workshop

Mary Wheeler, Director of The Center for Subsurface Modeling at University of Texas, Austin, and Phu Luong, ERDC On-Site EQM Lead, presented a computing portal for modeling multi-physics and multiple domains for environmental modeling at the NAVO MSRC PET training facility in March. A computational framework known as IPARS was presented that permits rigorous, physically representative coupling of different physical and numerical flow models in different parts of the domain on massively parallel systems or clusters of workstations. For more information on this workshop, visit

http://www.navo.hpc.mil/cgi-bin/pet/Training/training.cgi/

Sun's High Performance Computing Programming

This four-day workshop held in March presented programming techniques and skills to optimize and parallelize programs for the Sun Ultra Enterprise environment. Topics included Sun's Performance Workshop Tool Suite, Single Node/Single Process optimization, SGI to Sun porting issues, automatic and explicit parallelization, performance analysis of parallelized code, and optimizing and debugging MPI programs. In addition, an overview of the Sun MPI and cluster runtime programming environment was presented. For more information on this workshop, visit

http://www.navo.hpc.mil/cgi-bin/pet/Training/training.cgi/

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1-800-500-4722

Tiger Teams

Jay Boisseau, San Diego Supercomputer Center

INTRODUCTION

The San Diego Supercomputer Center (SDSC) is one of the NAVO MSRC PET academic affiliates. SDSC has been deeply involved with the NAVO MSRC PET program from the very beginning, and the scope of SDSC's involvement has increased each year in the program. The reason for SDSC's involvement has always been, and continues to be, to improve the computational infrastructure for scientific research at both NAVO and SDSC, thus making users at both sites more effective as scientists. This article describes the history of this involvement, the reasons it has been so successful, and some of the products of this valuable partnership. It closes with some comments on possible future interactions between SDSC and the NAVO MSRC.

SIMILAR MISSIONS AND USERS: LEVERAGING AND SYNERGY

Perhaps the primary reason that the partnership between SDSC and the NAVO MSRC has been so effective is that they have similar missions and goals. Both centers strive to increase scientific knowledge by making their researchers more effective through the application of advanced computing technologies. Both have large user communities of world-class scientists with varying degrees of computational expertise on HPC systems. Some of the areas of science even overlap: computational fluid dynamics is well represented in both user communities, as is research related to Earth systems sciences (climate/ocean modeling, weather forecasting, ground water modeling, etc.). SDSC and NAVO MSRC also have similar HPC resources, and their users face similar hurdles in developing high-performance parallel applications.

These commonalities have promoted the development of a unique relationship between SDSC, as an academic affiliate, and Logicon and the NAVO MSRC. SDSC, through its role as the leading-edge site in the National Partnership for Advanced Computational Infrastructure (NPACI), and Logicon, as the integrator for the NAVO MSRC, are developing comprehensive computational infrastructures that do more than just provide cycles. Their goals are to provide balanced archival storage hardware and networking capacity, and software technologies. They provide training to master these leading-edge hardware and software environments, which makes all of this easy to use effectively.

Advanced Visualization Systems (AVS) User Interface

SDSC has conducted a number of projects for Logicon and the NAVO MSRC (see next section) that also have value in the NPACI computational environments. The NAVO MSRC PET program enables the NAVO MSRC to leverage these SDSC/NPACI technologies, and in doing so accelerates their development by providing additional/supplementary funding to SDSC to develop, test, and implement these technologies. The results of these projects are implemented in both environments and therefore benefit both sets of users. More importantly, these projects benefit more researchers on a faster timescale than would be possible for either center to accomplish on its own. The resulting synergy enables both centers to fulfill their missions more effectively.

SDSC PROJECTS FOR NAVO PET

As stated above, SDSC proposes projects to Logicon that fulfill the mission of NAVO MSRC PET and also address NPACI strategic goals. Logicon reviews these projects and those proposed by other academic affiliates for their potential impact on the capabilities of NAVO MSRC users. Logicon then funds the projects deemed most likely to contribute to fulfilling the NAVO MSRC PET mission. In each of the first four years of the NAVO MSRC PET program, Logicon has selected SDSC to conduct a variety of projects. The selected projects leverage SDSC's expertise in a variety of computational areas, and the scope and funding of these activities have increased each year due to SDSC's successes. Some of these are noted in the following paragraphs; for more detailed information, please refer to the SDSC NAVO MSRC PET web pages: http://www.sdsc.edu/PET/NAVO

Tiger Teams

The most prominent project initiated by SDSC and Logicon has been the Tiger Team collaborations. SDSC and Logicon realized early on that the key to helping scientists overcome the steep learning curves associated with using new systems and software is often intensive, individual collaboration with computational experts who have already mastered these technologies. Tiger Teams are collaborations between SDSC computational experts and DoD scientists. NAVO MSRC PET Director Walter Shackelford, Computational Technology Area (CTA) Liaison Bob Melnik of Logicon, and NAVO MSRC PET Government Lead Eleanor Schroeder identify DoD researchers with strategic applications for participation in Tiger Team collaborations, while SDSC NAVO MSRC PET Lead Jay Boisseau identifies SDSC staff for participation. The SDSC staff come from computational science research backgrounds, but now focus on the application of advanced computing techniques to solve problems on HPC systems. They specialize in porting applications to leading-edge architectures and optimizing the computation and communications performance of these applications. They work with the selected DoD scientists, who have already made the transition to using HPC resources at the MSRC but who are more focused on the scientific techniques than on the HPC systems themselves. Thus, both parties are familiar with the specialties of the other, but each brings expertise to the table that can be combined to produce world-class scientific applications.

The Tiger Team approach has already achieved several notable successes. One particularly illustrative example of the power of this approach is the Tiger Team project on the CFDSHIP-IOWA code. Bob Sinkovits of SDSC worked with Eric Paterson of the University of Iowa and his team on optimizing the CFDSHIP-IOWA application for designing vessels on the T90 at NAVO MSRC and achieved better than a 2 times speed-up. This would have been a tremendous success on its own because the code was optimized and available for scientists to conduct more simulations. Sinkovits and Paterson carried the project even further, however, by teaming to develop a new parallel version of the code that tremendously increased the capability of future simulations in terms of both wallclock performance and available memory. The code has since been used in areas from computational fluid dynamics to environmental modeling by other researchers who had been waiting for a parallel version of this code to integrate into their research projects.

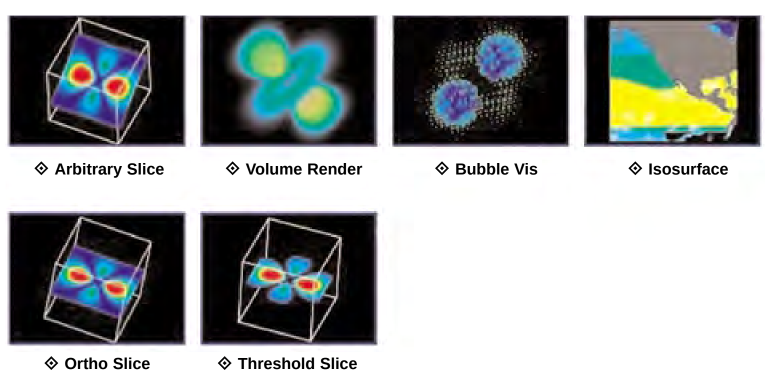
The Tiger Team approach has demonstrated many other successes in the past three years. These successes included: (1) optimizing the numerical flow algorithm (NFA) wake modeling code for the NAVO MSRC Cray T3E (Stuart Johnson of SDSC with Doug Dommermuth of Science Applications International Corporation (SAIC)), (2) optimizing the NOGAPS global weather prediction system (Giri Chukkapalli of SDSC with Tom Rosmond of NRL-Monterey), (3) optimizing the dieCAST regional ocean modeling code (Chukkapalli and Dongju Choi of SDSC with Steve Piacsek of NRL-Stennis), (4) developing a procedure for optimizing vector signal/image processing library (VISPL) routines for IBM SP and Cray T3E processors (Johnson with Rich Linderman of Wright Patterson Air Force Base (WPAFB)), and (5) providing external reviews and guidance to the developers of the MACH3D magnetohydrodynamics code (Tim Kaiser of SDSC with Bob Peterkin of Air Force Research Laboratory (AFRL)) and the FAST3D computational fluid dynamics code (Johnson with Jay Boris of NRL-Washington, DC). Current projects include optimizing the CH3D ground water modeling code (Sinkovits with Jeff Holland of ERDC) and the Coupled Ocean/Atmosphere Mesoscale Prediction (COAMPS) regional weather prediction code (Chukkapalli and Choi with Rich Hodur of NRL-Monterey).

Thus, while SDSC and other NAVO MSRC PET academic affiliates are working in specific projects to improve the ease of use as well as the effectiveness of the NAVO MSRC infrastructure (see next section), SDSC and Logicon initiated Tiger Teams with prominent DoD researchers to help them use resources that are currently still difficult to use effectively. Since HPC resources are

NAVO MSRC Visualization Lab

Visualization and Data Analysis Resource

Data Visualization Builder



VOLUME RENDER: The scalar value at each grid location in the 3D dataset is used as an index into a color/opacity lookup table. Each grid point is then rendered in 3D space as a region of the appropriate color and opacity.

always at the cutting edge, there will always be a need for both projects that make the resources easier to use and for Tiger Teams to help researchers master the issues and tasks that remain difficult to perform.

The Tiger Team program will be described in detail in future issues of *Navigator*, including individual articles on current and future collaborations.

Software Technology Projects

Most SDSC NAVO MSRC PET projects have been more "traditional" in the sense that they have funded the development and integration of software technologies into the NAVO MSRC environment to make it easier for scientists to use it more effectively. SDSC, in partnership with Oregon State University, provided the infrastructure to give web access to the operational status and queues on all NAVO MSRC machines. This project, led by Mary Thomas of SDSC, Ken Ferschweiler of Oregon State, and Andrew Schatzle of Logicon, enables users to quickly determine which systems are currently available and which queues are likely to yield the best turnaround times for jobs. Thus, a simple web page replaces several login sessions and interactive commands and has made using multiple NAVO MSRC systems much easier. This page is available now at http://www.navo.hpc.mil/Tools/Queues/.

Another web-based project designed to make MSRC facilities easier to use is PCOMP, the Parallel Computing Portal. PCOMP, led by Laura Nett of SDSC, is designed to help parallel application developers quickly find any source of general information on parallel computing, from web pages on programming tools (message passing interface (MPI), High Performance Fortran (HPF), etc.) to vendor documentation (Cray T3E, Sun HPC10000, IBM SP, etc.), to benchmarks, to HPC journals and newsletters. PCOMP complements the site-specific documentation provided by NAVO MSRC PET to assist the users with specific MSRC systems.

Scientific visualization is an important part of computational science, and SDSC has developed two projects designed to make MSRC visualization facilities easier to use. One is the Visualization and Data Analysis Resource, VADAR, developed by Greg Johnson of SDSC. It helps researchers learn to use the MSRC Visualization Center facilities to visualize their data in order to gain insight into the results of their simulations. It introduces them to the hardware and software available in the Vislab and guides them to the correct choices for the visualization needs. It then steps them through the process of visualizing their data, based on a series of simple questions. VADAR is available to NAVO MSRC users in the MSRC Visualization Center. The other web-based project designed to make the MSRC Visualization Center resources easier to use is the collaborative extension to the AVS available at http://www.navo.hpc.mil/cgi-bin/pet/Training/Resources/resources2.cgi?resource=avs, also developed by Greg Johnson. This tool makes it possible for researchers to explore their data visually over the Internet, sharing views of the visualizations that each party has the capability to alter. This can increase the tremendous productivity of colleagues at different locations working on the same project. Together, these tools enhance the overall productivity of MSRC users by enabling them to gain insight into their simulations more easily and rapidly.

An area of especially active collaboration between SDSC and NAVO MSRC has been security infrastructure. SDSC has long been recognized as a center of expertise in security technologies. The DoD MSRCs implement security measures to protect the integrity of the systems and of users' codes and data. Thus, this was a natural area of partnership and has been funded every year by Logicon. Tom Perrine of SDSC, a nationally recognized leader in computer security technologies, has worked on numerous security issues and projects, delivering expertise, white papers, and tools to the staff at the NAVO MSRC to provide a secure computing environment.

Finally, SDSC has contributed to a number of system-related projects that increase the functionality and robustness of NAVO MSRC systems. At the request of Northrop-Grumman, SDSC led a workshop for sites with large Cray T3Es to discuss a variety of system performance, security, and reliability issues. SDSC has responded to a number of other requests for advice on systems issues from NAVO MSRC staff. SDSC also participated in the porting and optimization of Legion for HPC systems, which has now been transferred to the MSRC staff.

Training

SDSC has participated in the NAVO MSRC PET Training Program as well as developing software technologies. An extremely comprehensive training program, led by Brian Tabor and Bob Melnik of Logicon, teaches users how to use MSRC facilities more effectively. SDSC has been asked to teach courses in parallel computing and in scientific visualization as part of this training program. Some of these classes are available for viewing on the Internet from the NAVO MSRC PET Training web pages http://www.navo.hpc.mil/cgi-bin/pet/Training/training.cgi . SDSC classes have been very well received, and the visualization classes in particular, taught by SDSC's Greg Johnson, are in high demand.

Supporting the Supercomputers

Part 1 of 2

By David Magee, Senior Systems Manager

In the supercomputing arena, the statistic that generally earns the largest headline is the peak FLOPS rating for a given system or center. However, successful implementation of multi-teraflop HPC systems and centers requires a clear balance of computational, mass storage, and networking capabilities—computing power has little value if commensurately robust storage and networks are not available. By the end of calendar year 1999, the Cray J916-based mass storage archival server at the NAVO MSRC was managing in excess of 160 terabytes of on-line storage. Current projections show a rapid expansion during calendar year 2000, approaching 400 terabytes by year's end! The planned upgrade of the Cray T3E to 1 teraflop and the addition of a 2-teraflop IBM SP require that we enhance our mass storage and network infrastructure to permit the most effective use of these systems, primarily by DoD Challenge projects and users.

In mid-1999, the NAVO MSRC began implementing significant improvements in its infrastructure in two concurrent projects. The first project was to design a resilient mass storage server capable of meeting current demands with the ability to scale and accommodate projected growth rates which will exceed 1 terabyte of new data per day with total archive capacities measured in petabytes. The second project was to reengineer the MSRC internal network to incorporate state-of-the-art networking technologies that provide unprecedented performance and resiliency.

Two Sun Microsystems, E10000s (E10Ks), were selected as the core hardware platform for the resilient mass storage server (RMSS). Storage and Archive Manager/ Quick File System (SAM-QFS) from LSC, Inc., was selected to provide a high-performance file system with robust and full-featured hierarchical storage management capabilities. The E10Ks share a large multi-terabyte array of fibre channel Redundant Array of Inexpensive Disks (RAIDs) capable of transfer speeds up to 100 megabytes per second per individual array. Multiple StorageTek (STK) robotic tape libraries are used to house the archive tape media and drives, which will include the new STK 9840 family of high-density, high-performance tape drives. In the event of a component (system, network, disk, tape drive, etc.) failure, Veritas Cluster software will facilitate the automated failover from one E10K system, component, or service to another, ensuring high availability and minimizing service interruptions to users. We believe this RMSS configuration will provide NAVO MSRC users with a scalable, robust, resilient mass storage server, using leading-edge technology to keep pace with the growing demand for data storage and retrieval. This

same configuration is being implemented at other DoD MSRCs and is expected to form the basis for a robust, common, wide-area RMSS capability across the DoD Shared Resource Centers.

In the next issue, Part 2 of this article will describe the ongoing NAVO MSRC network upgrades.

T3E Scalability

Dave Cole, NAVO MSRC Computer Systems and Support

DoD-wide demand for the NAVO MSRC Cray T3E system has been and remains extremely high, making it the most requested and successful scaleable parallel HPC system in the DoD HPC Modernization Program. In order to evaluate the T3E's ability to process even larger individual applications and aggregate workloads, it was temporarily upgraded in late November 1999 from 816 to 1,088 processors with an aggregate memory of approximately 400 gigabytes. This configuration positioned NAVO's T3E as the largest unclassified T3E in the world and number 8 in the Top 500 ranking.

The evaluation of the expanded T3E configuration ended in early February 2000 and was conducted in two phases. Phase 1 utilized existing challenge and non-challenge work to test aggregate workload scheduling with the primary goal of demonstrating a substantive improvement in system/job throughput as evidenced by a reduction in the general "expansion factors" for batch queues and queue complexes. No user action or intervention was required during this period of time.

Phase 2 consisted of scalability tests for selected applications that could effectively utilize much larger shares of T3E processor and memory resources. Phase 2 invitations were extended to all Computational Technical Area (CTA) leaders and to all DoD Challenge Project Principal Investigators (PIs) who were granted an FY2000 allocation on any DoD HPC system.

Four challenge projects representing three CTAs and two Services participated in the Phase 2 scalability tests and are listed in the table below. Members of the first two projects were unable to scale their code during the test period. The results from the two projects which successfully utilized the expanded T3E configuration, with comments by the respective PIs and/or authors, are available in the NAVO MSRC T3E Scalability Report.

Our analysis of Phase 1 utilization data for the months of October (before) and December (after) documents an increase in the number of jobs run, the capability to run large jobs, and better throughput as indicated by a decrease in the Normalized Expansion Factor. Phase 2 scalability test applications demonstrated the capability of the enhanced T3E to support world-class high performance computing. A 1/32-degree near-global simulation, which typically uses 474 processors, was run on 948 processors. The decrease in run time from 14.35 hours to 8.35 hours achieved a near linear speed up of the finest resolution global ocean model.

Benchmark tests using 1,024 processors included 1.02-billion-atom Molecular Dynamics simulation and 22,500-atom Quantum Molecular Dynamics simulations within the Density Functional Theory—the largest classical and quantum molecular-dynamics systems simulation in history. Additionally, aggregate workload handling was vastly improved, thereby demonstrating a capacity solution in addition to an unparalleled DoD HPC single system capability. T3E usage during the test period is a clear indicator of the need for scaleable parallel-distributed memory HPC systems of this size.

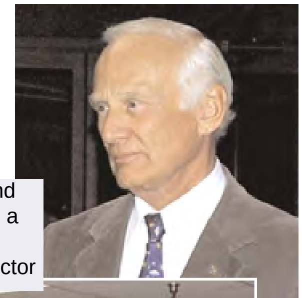
The NAVO MSRC gratefully acknowledges the hardware, software, and support provided by SGI and Logicon Inc., which made the T3E test and evaluation possible. We would also like to thank all Challenge team members who participated in the Phase 2 scalability tests for their time and efforts.

CTA	Service	Project
CFD	Air Force	Unsteady Aerodynamics of Aircraft Maneuvering at High Angles of Attack
CCM	Air Force	Design of New Materials Using Computational Chemistry
CCM	Air Force	Computational Assisted Development of High Temperature Structural Materials
CWO	Navy	Global and Basin-Scale Ocean Modeling and Prediction

A Look Inside NAVO MSRC

We welcome our visitors...

George Walker, Chairman of the State Board for Junior and Community Colleges; Lois McMurchy, Director of the Skill Technology Center, Coahoma Community College; and RADM Paul G. Gaffney, Chief of Naval Research, visit the NAVO MSRC booth at the JASON XII Exhibit at Coahoma Community College, Clarksdale, Mississippi



Dr. Buzz Aldrin, Gemini and Apollo Astronaut, receives a tour from Terry Blanchard, NAVO MSRC Deputy Director

Challenge Researchers, Eric Chassignet and Remy Baraille, receive a tour of operations from Scientific Visualization Staff, Pete Gruzinskas and Andy Haas

Left to right: Ms. Susan Butler, Legislative Staff Member; CAPT Larry Warrenfeltz, Commanding Officer, Naval Oceanographic Office; Dr. Vance Coffman, Chief Executive Officer, Lockheed Martin; Mr. Eric Womble, Legislative Staff Member; Congressman Chip Pickering, 3rd District, State of Mississippi; Mr. Jim Sartucci, Legislative Director for Senator Trent Lott; Sonny Montgomery, Former Congressman, State of Mississippi; RADM Kenneth Barbor, Commander, Naval Meteorology and Oceanography Command

Steve Adamec, NAVO MSRC Center Director, and Congressman Chip Pickering, 3rd District, State of Mississippi

Navigator Tools and Tips

Quotas

Sheila Carbonette, User Services

Users are allocated a home directory on each NAVO MSRC system with a certain amount of permanent non-migrated storage. Disk quotas on these home directories are enforced to prevent the system's disks from becoming full. The current home directory quotas are listed below:

System	Maximum Size of $HOME (in megabytes)
T3E (seymour)	250
T90 (neptune)	250
SV-1 (poseidon)	250
O2K (odyssey)	500

The "quota -v" command can be used to display users' disk usage and limits even if they have not been exceeded. The output from this command ran on the T3E (seymour) and Origin 2000 (odyssey) will look similar to the following example for a UNICOS system:

```
seymour% quota -v
File system: /u/home
User: shecar, Id: 214
                      File blocks (512 bytes)        Inodes
=============================================================
User Quota:           512000* ( 69.2%)              Unlimited*
Warning:              460800* ( 76.8%)              None
Usage:                354048                        928
```

The "File blocks" column shows the quota block counts and block usage for online quotas. All values are measured in 512-byte blocks. The "Inodes" column relates to inode quotas and these quotas are not implemented on the UNICOS systems. The "User Quota" row shows a user's current disk quota. The "Usage" row shows how much disk space the user's home directory is currently using. The following is an example for an IRIX system:

```
odyssey% quota -v
Disk quotas for shecar (uid 214):

Filesystem  usage   quota   limit   timeleft  files  quota  limit  timeleft
=============================================================================
/tmp        36      0       0       11        0      0      0      0
/scr        8       0       0       18        0      0      0      0
/u/home     511880  512000  512000  1699      0      0      0      0
```

The "usage" column shows how much disk space the user's home directory is currently using. The "quota" column shows a user's current disk quota. The "limit" column shows the maximum amount of disk space a user's account can use. The remaining columns relate to inode quotas, and these quotas are not implemented on the IRIX systems. All values are measured in kilobytes. The /tmp and /scr filesystems are for information purposes only. Quotas are not implemented on these systems.

Upcoming Events

June 4-7, 2000
User's Group Conference
Albuquerque, NM

June 19-22, 2000
Government Technet 2000 Conference
DC Convention Center
Washington, DC

July 23-28, 2000
SIGGRAPH 2000
New Orleans, LA
www.siggraph.org/

November 4-10, 2000
Supercomputing '00
Dallas, TX
www.sc00.org/

November 28 - December 2, 2000
IEEE International Conference on Cluster Computing CLUSTER 2000 Germany
www.tuchemnitz.de/informatik/RA/cluster2000/

Recent Events

The C90 Retires

Former and current NAVO MSRC Center Directors, Terry Blanchard, Cecil Watkins, Steve Adamec, and Dan Williams

A panamoric view in the operations center of the C90 being de-installed

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